REPORT DOCUMENTATION PAGE

1

Form Approved OMB NO. 0704-0188

1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE	3. DATES COVERED (From - To)
24-09-2014	Final Report	7-Aug-2012 - 6-Oct-2014

4. TITLE AND SUBTITLE
Final Report: Computing Environment for Adaptive Multiscale Simulation

5a. CONTRACT NUMBER
W911NF-12-1-0371

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER
611103

6. AUTHORS
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5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAMES AND ADDRESSES
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8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS (ES)
U.S. Army Research Office
P.O. Box 12211
Research Triangle Park, NC 27709-2211

10. SPONSOR/MONITOR'S ACRONYM(S)
ARO

11. SPONSOR/MONITOR'S REPORT NUMBER(S)
61446-MA-RIP.1

12. DISTRIBUTION AVAILIBILITY STATEMENT
Approved for Public Release; Distribution Unlimited

13. SUPPLEMENTARY NOTES
The views, opinions and/or findings contained in this report are those of the author(s) and should not contrued as an official Department of the Army position, policy or decision, unless so designated by other documentation.

14. ABSTRACT
This DURIP project was used to upgrade the computing capabilities of Rensselaer's Scientific Computation Research Center (SCOREC). The primary component is a parallel computing cluster with 22 Dell R620 compute nodes, each with two 8-core 2.6 GHz Intel Xeon processors (352 processors) and a direct connection to both a 56Gbps Infiniband fabric and a 10Gbps Ethernet fabric. To support the I/O demands storage arrays of 110 teraflops have been added to the SCOREC system. The last component is four workstations with an Intel Core i7 3.6 GHz 4-core processor and a Nvidia GTX580 graphics card.

15. SUBJECT TERMS
Parallel computing cluster, High performance computing

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
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UU	UU	UU	UU		19b. TELEPHONE NUMBER 518-276-8044

Report Title

Final Report: Computing Environment for Adaptive Multiscale Simulation

ABSTRACT

This DURIP project was used to upgrade the computing capabilities of Rensselaer's Scientific Computation Research Center (SCOREC). The primary component is a parallel computing cluster with 22 Dell R620 compute nodes, each with two 8-core 2.6 GHz Intel Xeon processors (352 processors) and a direct connection to both a 56Gbps Infiniband fabric and a 10Gbps Ethernet fabric. To support the I/O demands storage arrays of 110 teraflops have been added to the SCOREC system. The last component is four workstations with an Intel Core i7 3.6 GHz 4-core processor and a Nvidia GTX580 graphics card.

These systems upgrades are being used to support two ARO grants (i) "Multiscale Modeling of the Mechanics of Advanced Energetic Materials Relevant to Detonation Prediction" (W911NF-09-1-0330) and (i) "Methods for the Reliable Simulation of Multiphase Processes" (W911WF-14-1-0301), and the RPI subcontract to an SBIR entitled "Mesh Generation and Control for Moving Boundary Problems" in support of the Coastal & Hydraulics Laboratory of the US Army Corps of Engineers.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received Paper

TOTAL:

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received Paper

TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Number of Presentations: 0.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received Paper

TOTAL:

Number of Manuscripts:

Books

Received Book

TOTAL:

Received Book Chapter

TOTAL:

Patents Submitted

Patents Awarded

Awards

Graduate Students

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:..... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):..... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields: 0.00

Names of Personnel receiving masters degrees

NAME

Total Number:

Names of personnel receiving PHDs

NAME

Total Number:

Names of other research staff

NAME PERCENT_SUPPORTED

FTE Equivalent:
Total Number:

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

Technology Transfer

Computing Environment for Adaptive Multiscale Simulation W911NF-12-1-0371

Introduction

This DURIP project provided funds for computing hardware to upgrade the computing capabilities of Rensselaer's Scientific Computation Research Center (SCOREC). The primary driver for the requested system at the time of the DURIP proposal submission was our ongoing U.S. Army Research Office grant entitled "Multiscale Modeling of the Mechanics of Advanced Energetic Materials Relevant to Detonation Prediction", W911NF-09-1-0330, Professors Catalin R. Picu and Mark S. Shephard, Principal Investigators. As indicated below, this system is being effectively applied to the needs of that, and other multiscale computation projects. As of September 15, 2014, this systems is also supporting much of the computational needs of our new U.S. Army Research Office grant entitled "Multiscale Methods for the Reliable Simulation of Multiphase Processes", W911WF-14-1-0301, Professors Assad A. Oberai, Onkar Sahni and Mark S. Shephard, Principal Investigators. The systems is also supports development efforts on the RPI SCOREC subcontract to an SBIR entitled "Mesh Generation and Control for Moving Boundary Problems" in support of the Coastal & Hydraulics Laboratory of the US Army Corps of Engineers.

Computing System Upgrades Support by DURIP

The funds from the DURIP grant supported the purchase of (i) a parallel computing cluster, (ii) an extension to the SCOREC data servers and storage system, (iii) a new network switch and (iv) high end graphics workstations.

Parallel Compute Cluster: The parallel compute cluster purchased with the DURIP funds consists of 22 Dell R620 compute nodes, each with two 8-core 2.6 GHz Intel Xeon processors, 128 GB of DDR3 1600MHz RAM, and a direct connection to both a 56Gbps Infiniband fabric and a 10Gbps Ethernet fabric. We expect each node to peak at about 320 GigaFLOPS, with an aggregate performance about 7 TeraFLOPS. To be able to do larger problems, the 22 nodes have been integrated with others purchased by RPI to form a larger cluster totaling 64 nodes of the same specification, with an aggregate performance of 20 TeraFLOPS. Although this combined system is accessible to others, each of the three groups that contributed has full access to at least their portion of the system any time they require it and can access more than that portion at times those nodes are not in use.

Data Servers and Stotage: To handle the increased I/O demands, we have added a 96 terabyte array and a 14 terabyte array. The 96 terabyte array handles most data for the cluster, while the 14 terabyte array is storing code, applications, and other resources used by the cluster. Both arrays are built on two 6-core 2.6 GHz Xeon Processors, with 128 gigabytes of RAM. The 96 terabyte array consists of 24 4 terabyte SAS drives and the 14 TB array consists of 24 600 gigabyte 10,000 RPM SAS disks. Each array is capable of sustaining transfer speeds of over 1 Gigabyte/second and are connected to a 10Gbps Ethernet Fabric.

Network Switch: The 10-Gigabit Ethernet fabric is now being supported by an Arista 7150S, 24-port Layer-3 switch along with Intel x520-DA2 network interface cards, which significantly increases our data transfer throughput internally. Additionally, we upgraded our uplink to campus to match the new capabilities of the switch.

Workstations: Four high-end graphics workstations that greatly increase our ability to prepare simulations, develop code, and visualize results were also added to the SCOREC system as part of this project. Each workstation has an Intel Core i7 3.6 GHz 4-core processor, 32 GB of DDR3 1600MHz RAM, and 2GB Nvidia GTX580 graphics card driving a 30" Dell Ultrasharp 2560x1600 resolution monitor.

Application to Multiscale Computations

The central focus of our original ARO grant is the simulation of the plasticity of the energetic material RDX. Figure 1 shows a projection of the RDX crystal containing a dislocation gliding on one of the horizontal atomic planes. The defects of this crystal are believed to play a central role in detonation initiation. Detailed molecular studies are used to study these mechanisms. A typical simulation includes about 2000 molecules and requires a time step of 2.35E6 fs. On the new cluster such models require 3 to 9 hours each using all 352 cores.

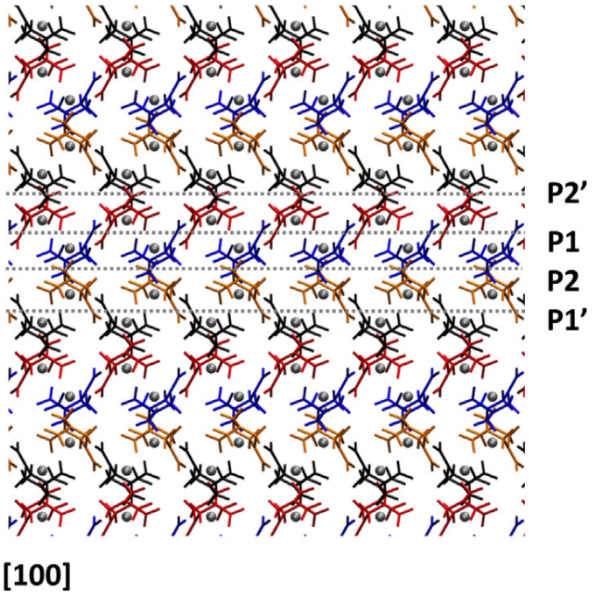


Fig. 1. [001] projection of a RDX crystal.

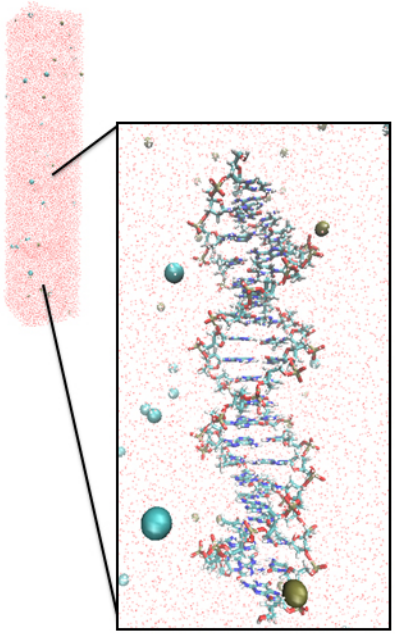


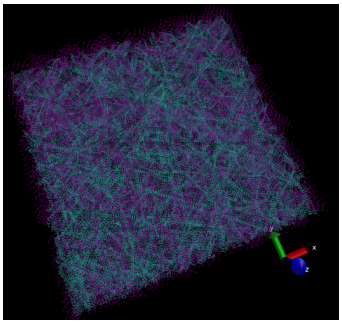
Fig. 2. DNA strand embedded in an ionic solution.

Molecular dynamics is also used to model the mechanics of DNA strands with full atomistic detail. The objective of this work is to quantify the strength of DNA junctions; such junctions stabilize DNA crystals. The strength cannot be measured directly since manipulation of individual DNA strands is not straightforward. Therefore, simulations such as the ones we perform are the only means to obtain order of magnitude estimates of such parameters. The values are then used to engineer DNA crystals and their

production process. Fig. 2 shows a DNA strand in an ionic solution. These simulations typically use 100,000 atoms and 10,000,000 time steps per stretch test. A single simulation requires 24 hours to execute.

Fibrous materials are ubiquitous in everyday life, in engineering and biology. All such fiber networks have some degree of randomness and this aspect imparts special properties to the ensemble. Furthermore most are composites in the sense that either or both are made from fibers with various properties and embed inclusions of various sizes and shapes. We use large scale simulations to represent the deformation and failure of such structures.

The deformation of collagen networks, relevant for tissue mechanics, is modeled using large models of random fiber networks. Models of complex networks of polymeric fibers such as that shown in Fig. 3 are developed and used to represent components material systems. Other simplified networks such as those shown in Fig. 4, in both 2D and 3D are used for more theoretical purposes and to gain insights into various specific features of the mechanics. Although the individual simulations only require modest parallel compute power, on the order of 500 replicas are required to be statically meaningful.



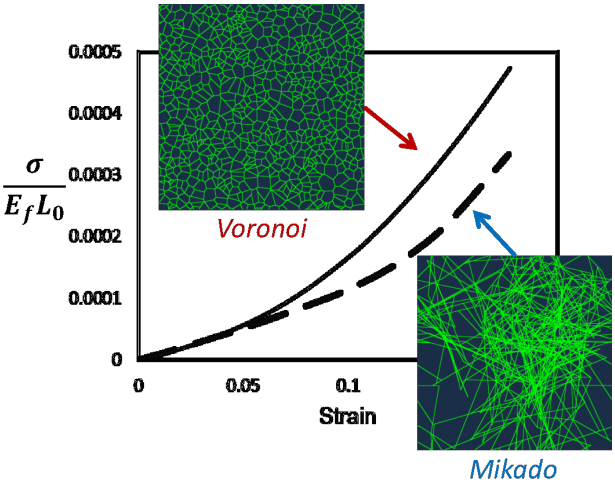


Fig. 3. Mat of polymeric fibers. Fig. 4. 2D models of networks and their stress-strain curves.

Application on New Projects

Our new ARO supported grant entitled “Multiscale Methods for the Reliable Simulation of Multiphase Processes” is focused on the developing mathematical and computational modeling strategies for solving multiphase problems including ones involving chemically reacting phases at the interfaces, and problems with three phases and contact lines. In order to solve these problems we propose thermodynamically consistent mathematical models and accompanying adaptive discretization methods. Further, these problems require an accurate geometric representation of the interface between phases (in order to model the chemical reactions that occurs at the interface, and to accurately represent the curvature which is critical in the contact line problem). Therefore we will develop novel, highly accurate interface tracking methods that will be implemented in an infrastructure that supports the proposed adaptive simulations. The DURIP support systems will be central to the development,

testing and initial scaling of the methods and associated software. The complete simulations will require execution on substantially larger massively parallel systems.

The RPI SCOREC efforts on the SBIR entitled “Mesh Generation and Control for Moving Boundary Problems” are focused on bringing our parallel unstructured mesh technologies to the adaptive solution of large scale multiphase flow problems of importance to the Coastal & Hydraulics Laboratory of the US Army Corps of Engineers. The SCOREC team is providing the parallel mesh infrastructure, parallel mesh adaptation software and is coordinating with researchers at the Coastal & Hydraulics Laboratory on the development of the discretization error estimators and adaptive mesh control strategies. The DURIP systems will be central to the development, testing and initial scaling of the methods and associated software developed in this project.